

# Interface states in bilayer graphene and valleytronics

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## Abstract

We study the states localized near an interface between conducting and insulating bilayer graphene (BLG) and show that they have highly unusual properties that have no analog in conventional systems. Moreover, the states belonging to the two independent valleys in the Brillouin zone of BLG show contrasting properties that allow an *easy* experimental realization of various valley based functionalities desired in valleytronics *without* requiring any sophisticated techniques.

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Bilayer graphene— two layers of carbon atoms with the same intralayer arrangement of atoms and relative stacking of the layers as in natural graphite, is focus of intensive experimental and theoretical research these days due to its unusual physical properties[1–8]. There are two independent valleys in Brillouin zone of BLG and the low energy elementary excitations in both valleys posses a pseudospin and have pseudospinor wavefunctions. The valley degree of freedom can be used for controlling an electronic device similar to the spin or charge and there are many proposals for achieving basic functionalities desired in this field, named valleytronics, using graphene systems[9–14]. In ref[10], A. Rycerz et. al. proposed a valley filter that is a strip of monolayer graphene containing a narrow constriction with zigzag edges. However, experimental realization of such a device is challenging, if not impossible. Taking advantage of the effects of trigonal warping at high carrier densities in monolayer graphene, J. L. Garcia-Pomar et. al.[11] proposed a device which again requires zigzag edges in addition to manipulation of beams of particles— again a great challenge to the experiment. In bilayer graphene, A. S. Moskalenko and J. Berakdar[12] showed that intense *shaped* light pulse can induce valley polarized currents and, D. S. L. Abergel and Tapash Chakraborty[13] proposed a device for generating valley polarized currents where in the presence of an intense terahertz light source in a region of bilayer graphene with a finite band gap the dynamically induced states can be made to exist only in a given valley by tuning different parameters. Although, these are relatively easy for experimental tests, they are hard to implement in practical devices. H. Schomerus’ proposal[14] uses the fact that the angular dependence of the transmission probabilities of the particles of the two valleys from one region to another differ when the two regions have opposite pseudospin polarization. It demands a relatively sharp fermi surface and again controlling beams of particles and their propagation angles. Here we show that states that are localized near an interface of zero band gap and finite band gap BLG have highly unusual properties that provide us with a conceptually extremely simple way of obtaining valley polarization and related basic functionalities, and eliminate almost all experimental challenges that stand in the way of valleytronic devices.

In a clean zero band gap or conducting BLG at any energy there are two pseudospinor plane wave states and two pseudospinor evanescent wave states. The latter have appreciable magnitudes only near interfaces between regions of different potentials and play an important role in transport properties. Similar is the case of a clean finite band gap or insulating BLG

where the evanescent waves are localized near interfaces between regions of different band gaps or potentials. For the first case they are only present at energies which are outside the band gap of at least one side. For energies outside band gap these states have the usual properties, however, for energies inside the band gap, their wavevectors become complex so the spatial parts of their wavefunctions contain plane waves as well as evanescent ones. This is unusual for any wave in a pristine and dissipation-free system and here it is more unusual as it apparently shows that number of particles is not conserved. In search of resolution to this issue we derive the continuity equation associated with the Hamiltonian of the system and check the current these states carry along the decay direction. It comes out to be *zero* just like the usual evanescent waves which is quite interesting. However, these states show a more interesting behavior in the transverse direction: the states belonging to the two valleys carry currents in *opposite* and *fixed* directions, *independent* of the sign of the wavevector component along this direction. The latter property is in stark contrast to common systems described by the usual Schrodinger wave equation. For an interface of a conducting and insulating BLG, due to the continuity of probability current density, these states modifies the behavior of the states localized on the conducting side as well. Thus the particles of a given valley in conducting region at *any energy* inside the band gap of the insulating BLG coming towards the interface at *any angle* turn towards *the same* lateral side close to the interface. Thus without worrying about the propagation angles of the quasiparticles or the finite smearing of the fermi surface due to temperature or any other intravalley scatterings, we can easily separate particles of the two valleys and also perform other valley based operations just by using a simple junction of conducting and insulating BLG either in above mentioned geometry or by applying a voltage difference along it as proposed in ref[9] for the topologically confined zero energy chiral modes.

The low energy electronics properties of the BLG system lying in the xy-plane can be approximately described by effective Hamiltonians  $H^\pm$  for the two valleys  $K(+)$  and  $K'(-)$  [7, 8] which along with their pseudospinor eigenfunctions  $\Psi^\pm(x, y)$  can be written as

$$H^\pm = \begin{pmatrix} -U & \nabla_\mp \\ \nabla_\pm & U \end{pmatrix}, \Psi^\pm(x, y) = \begin{pmatrix} \varphi_A^\pm \\ \varphi_B^\pm \end{pmatrix} \quad (1)$$

Where the components  $\varphi_A^\pm$  and  $\varphi_B^\pm$  of  $\Psi^\pm(x, y)$  are envelope functions that give the amplitudes on the two different layers on sites A and B that do not lie directly above or

below sites on the other layer.  $\nabla_{\pm} = \frac{\hbar^2}{2m}(\partial_x \pm i\partial_y)^2$  where  $\partial_{x,y}$  are differential operators, the two layers have on-site energies equal to  $\pm U$  induced by applied electrostatic gates, and  $m$  is the effective mass of quasiparticles when  $U = 0$ . When  $U \neq 0$  inversion symmetry between the two layers is broken and a band gap equal to  $2|U|$  is produced. Dispersion for both valleys is the same and reads:  $E(\mathbf{k}) = \pm \sqrt{U^2 + (\frac{\hbar^2 k^2}{2m})^2}$  where  $\pm$  refer to electron and hole bands here. Suppose an interface between conducting region (CR,  $x < 0$ ) and insulating region (IR,  $x > 0$ ) of BLG at  $x = 0$  then  $U = 0$  for  $x < 0$  and we have continuum of propagating and evanescent states in CR while in IR for energies inside the gap only the states localized near the interface are present. The states in CR match those in the IR with the same energy  $E$  and, due to the invariance along the interface, with the same y-component of wavevector  $k_y$  to ensure the continuity of the probability density and the probability flux density. Thus we can use  $E$  and  $k_y$  to label all the states. In IR, for a given  $E$  and  $k_y$ , the x-components of wavevectors  $\pm k_x$  are complex quantities given by  $k_x = \pm k_r + ik_i$  where  $k_r = \eta \sin \alpha$  and  $k_i = \eta \cos \alpha$ , and we defined  $\eta = (\delta^2 + k_y^4)^{1/4}$ ,  $\alpha = \frac{1}{2} \tan^{-1}(\delta/k_y^2)$  and  $\delta = \sqrt{U^2 - E^2}$ . For simplicity we absorbed  $\frac{2m}{\hbar^2}$  in energy terms and we will do so hereafter. This results in *decaying plane waves*. The wavefunctions of the states belonging to the two valleys are  $\Psi_2^{\pm}(x, y) = \Psi_2^{\pm}(x)e^{ik_y y}$  where, ignoring the solutions that diverge with  $x$ ,  $\Psi_2^{\pm}(x)$  are given by

$$\Psi_2^{\pm}(x) = a_2^{\pm} \begin{pmatrix} \frac{E-U}{\Omega_{\pm}} \\ -\frac{R_{\pm}}{\Omega_{\pm}} e^{2i\theta_{\pm}} \end{pmatrix} e^{ik_r x - k_i x} + d_2^{\pm} \begin{pmatrix} \frac{E-U}{\Omega_{\pm}} \\ -\frac{R_{\pm}}{\Omega_{\pm}} e^{-2i\theta_{\pm}} \end{pmatrix} e^{-ik_r x - k_i x} \quad (2)$$

Here  $a_2^{\pm}$  and  $d_2^{\pm}$  are complex coefficients determined by matching conditions,  $R_{\pm} = k_r^2 + (k_i \pm k_y)^2$ ,  $\Omega_{\pm} = \sqrt{(E - U)^2 + R_{\pm}^2}$  and  $\theta_{\pm} = \tan^{-1}(\frac{k_i \pm k_y}{k_r})$ . The spatial parts of the above wavefunctions apparently show currents along  $\pm x$  with magnitudes decreasing with  $x$ , however, as we will shortly confirm, the relative phases  $\pm 2\theta_{\pm}$  between upper and lower components of the pseudospinors contain the information needed to produce the proper results. We derive expressions for probability current densities  $\mathbf{J}^{\pm}$  for the two valleys associated with the Hamiltonians  $H^{\pm}$  in equation 1, they read:  $\mathbf{J}^{\pm} = (J_x^{\pm}, J_y^{\pm})$  where  $J_x^{\pm}$  and  $J_y^{\pm}$  are given by

$$J_x^{\pm} = \frac{-\hbar}{m} \{ \text{Im}(\Psi^{\dagger} \sigma_x \partial_x \Psi \pm \Psi^{\dagger} \sigma_y \partial_y \Psi) \}$$

$$J_y^{\pm} = \frac{-\hbar}{m} \{ \text{Im}(-\Psi^{\dagger} \sigma_x \partial_y \Psi \pm \Psi^{\dagger} \sigma_y \partial_x \Psi) \}$$

Here  $\sigma_{x,y}$  are Pauli's matrices. It is also worth mentioning that these expressions show that unlike common systems the continuity of flux density is ensured with that of wavefunction and its first derivative in spite of the fact that in case of finite band gap BLG we have energy dependant effective mass as is clear from the dispersion relation. Further, the mixed  $x, y$  terms shows some intimate link between the two orthogonal directions. Using these expressions and defining  $\beta = \tan^{-1}(\frac{k_y}{k_x})$  the angle that  $\mathbf{q} = (k_x, k_y)$  makes with the x-axis, it is straightforward to show that the currents  $\mathbf{J}_2^\pm = (J_{2x}^\pm, J_{2y}^\pm)$  carried by  $\Psi_2^\pm(x)$  are

$$\begin{aligned} J_{2x}^\pm &= -C^\pm (|a_2^\pm|^2 - |d_2^\pm|^2) q \cos(2\theta_\pm \mp \beta) e^{-2k_x x} \\ J_{2y}^\pm &= C^\pm \{ \mp (|a_2^\pm|^2 + |d_2^\pm|^2) q \sin(2\theta_\pm \mp \beta) + 2k_y \operatorname{Re}(a_2^\pm d_2^{\pm*} e^{2i(\theta_\pm + k_x x)}) \} e^{-2k_x x} \end{aligned}$$

where  $C^\pm = \frac{\hbar}{m} \frac{(U-E)R_\pm}{\Omega_\pm^2}$ ,  $q = |\mathbf{q}|$  and  $*$  shows complex conjugation. Note that the cross terms in  $J_{2x}^\pm$  vanish. Using a few common trigonometric identities we get  $2\theta_\pm \mp \beta = \pi/2$  independent of any parameter so *both* terms in  $J_x^{\pm a}$  vanish to give

$$J_x^{\pm a} = 0$$

Thus the relative phases between components of pseudospinors count for the presence of plane waves and we obtain sensible results. A more interesting result is the currents along y-direction:

$$\begin{aligned} J_{2y}^\pm &= C^\pm \{ \mp (|a_2^\pm|^2 + |d_2^\pm|^2) q + 2k_y \operatorname{Re}(a_2^\pm d_2^{\pm*} e^{2i(\theta_\pm + k_x x)}) \} e^{-2k_x x} \\ &= C^\pm \{ \mp (|a_2^\pm|^2 + |d_2^\pm|^2) \sqrt{k_y^2 + k_x^2} + 2 |a_2^\pm| |d_2^\pm| k_y \cos(2\theta_\pm + 2k_x x + \phi_a^\pm - \phi_d^\pm) \} \end{aligned}$$

where  $\phi_p^\pm = \operatorname{Arg}(p_2^\pm)$  ( $p = a, d$ ). Above expressions contain a wealth of information. It is not difficult to see that for any values of coefficients  $a_2^\pm$  and  $d_2^\pm$  the first term always dominates so the currents of the two valleys are not only in opposite directions, their directions are fixed and do not change with sign of  $k_y$ . This is unusual and unlike the case of ordinary systems described by usual Schrodinger equation where in case of invariance along y-direction y-component of current  $J_y^S$  always follow the sign of the  $k_y$  and can always be written as  $J_y^S = \frac{\hbar k_y}{m} \rho(x)$  where  $\rho(x)$  is probability density and other factors have obvious meanings. Above result shows that, on one hand we can use these states for valley dependant functionalities by applying a voltage difference along the interface and on other hand,

coupled with the fact that current has to be continuous at the interface it implies that the states of the two valleys in CR propagating towards the interface at any positive or negative angle will carry currents in the same fixed directions close to the interface on its *both* sides. Far from the interface in CR flux have to follow the sign of  $k_y$ . The strip-like region around the interface where valley dependant properties show up are defined by localization lengths of the evanescent states on both sides. This also shows that the localized states in IR at  $E$  inside the band gap modify the behavior of those in CR that usually do not distinguish between the two valleys and currents carried by them follow the sign of  $k_y$ . Another interesting point is that  $J_{2y}^\pm$  is non-zero even when  $k_y = 0$  and more important for practical purposes is that the factors  $C^\pm$  switch sign with the polarity of the gates. This is clear from their expressions where all terms on right side are positive definite except  $(U - E)$  which is positive for  $U > 0$  and negative otherwise. Thus we can control the directions of the currents of the two valleys with the polarity of the gates. This broadens the possible set of functionalities we can achieve using these states. Further, since all states with energy inside the band gap have similar behavior, smearing of fermi surface due to temperature or any intravalley scatterings, which are almost unavoidable in real systems, is harmless so experimental realization of a device where valley based operations could be performed is expected to be very simple and easy using these localized states. One way is, similar to ref[9] as mentioned earlier, to use just the narrow strip region of the interface where a small voltage difference along it can be used to get a net valley polarized current or filter a valley which can be of particles belonging to either valley depending on the polarity of gates used to create the band gap. Two such set ups in series can be used as a valley valve where particles can only pass if the polarities of the gates are the same for the two. Another way is to use the CR as the source of particles and again in this case depending on the polarity of the gates one of the contacts on the lateral sides will collect only particles of one valley. These contacts do not need to be very fine on the IR, however, they must not extend in CR more than the localized states otherwise they will also collect particles of the other valley. And similar to the above case a combinations of such set ups can be used for other functionalities.

For completeness, let's compute the currents  $J_{2y}^\pm$  carried by the localized states on IR as well as the currents along the interface  $J_{1y}^\pm$  in CR when the particles in CR travel towards the interface at a positive energy  $E$  and with y-component of wavevector  $k_y$ . The

wavefunctions in CR in this case can be written as  $\Psi_1^\pm(x, y) = \Psi_1^\pm(x)e^{ik_y y}$  with  $\Psi_1^\pm(x) = \begin{pmatrix} 1 \\ -e^{\pm 2i\phi} \end{pmatrix} e^{+ikx} + b_1^\pm \begin{pmatrix} 1 \\ -e^{\mp 2i\phi} \end{pmatrix} e^{-ikx} + c_1^\pm \begin{pmatrix} 1 \\ h^\pm \end{pmatrix} e^{+\kappa x}$  where  $b_1^\pm$  and  $c_1^\pm$  are complex coefficients,  $h^\pm = (\sqrt{1 + \sin^2 \phi \mp \sin \phi})^2 = 1/h^\mp$ ,  $k = \sqrt{E - k_y^2}$ ,  $\kappa = \sqrt{E + k_y^2}$  and  $\phi = \tan^{-1}(\frac{k_y}{k})$ . Using the matching conditions  $\Psi_1^\pm(x=0) = \Psi_2^\pm(x=0)$  and  $\partial_x \Psi_1^\pm(x)|_{x=0} = \partial_x \Psi_2^\pm(x)|_{x=0}$  we determine all the coefficients  $b_1^\pm, c_1^\pm, a_2^\pm$  and  $d_2^\pm$ . As expected for energies inside the band gap,  $|b_1^\pm| = 1$  so there is no net current along x-direction. Further, we find that  $|a_2^\pm| = |d_2^\pm| \equiv |a^\pm|$  so we can write  $J_{2y}^\pm = 2\frac{\hbar|k_y|}{m} \frac{(U-E)R_\pm}{\Omega_\pm^2} |a^\pm|^2 \{\mp \sqrt{1 + (k_r/k_y)^2} + \text{sgn}(k_y) \cos(2\theta_\pm + 2k_r x + \phi_a^\pm - \phi_d^\pm)\} e^{-2k_i x}$ . This expression clearly shows the independence of directions of  $J_{2y}^\pm$  from the sign of  $k_y$  and other features mentioned above. Currents of the two valleys in CR  $J_{1y}^\pm$  are determined by using  $\Psi_1^\pm(x, y)$  with above calculated coefficients  $b_1^\pm$  and  $c_1^\pm$ . Figure(1) shows the contour plots of the currents of the two valleys along the y-direction  $J_y^\pm$ , where  $J_y^\pm$  equals  $J_{1y}^\pm$  for  $x < 0$  and  $J_{2y}^\pm$  otherwise, for  $E = 17\text{meV}$  and  $U = \pm 50\text{meV}$  as a function of  $k_y$  and distance from the interface. Purple (dark) and off-white (bright) colors show currents along  $-\hat{y}$  and  $+\hat{y}$  respectively. Figures(1a,b) show  $J_y^\pm$  for  $U = \pm 50\text{meV}$  and  $U = \mp 50\text{meV}$ , also indicating that  $J_y^+$  is the same for a given polarity of gates as  $J_y^-$  for the opposite polarity and this relation holds at all positions  $x$  and for all values of  $k_y$ . It is clear that for  $U = +50\text{meV}$ , close to the interface,  $J_y^+$  flows towards  $-\hat{y}$  for all possible *positive* and negative values of  $k_y$  where as  $J_y^-$  flows towards  $+\hat{y}$  for all possible positive and *negative* values of  $k_y$ . Further, for the opposite polarity of gates, i.e., for  $U = -50\text{meV}$ , currents of both valleys switch directions. From the figure, the width of the strip-like region where this behavior is observed is approximately  $15\text{nm}$  for the parameters used so for an interface sharp enough that these localized states can be used but smooth enough that intervalley scatterings can be ignored is clearly possible. Far from the interface currents for the two valleys retain the usual behavior. In IR they vanish when  $k_i x \gg 1$  where as in CR for  $\kappa|x| \gg 1$  their directions follow the sign of  $k_y$ . We can also see this fact by calculating  $J_{1y}^\pm$  far from the interface where the localized states have negligible effects. They are given by  $J_{1y}^\pm = \frac{4\hbar k_y}{m} \{1 - \cos(2kx - 2\phi - \phi_b^\pm)\}$  where  $\phi_b^\pm = \text{Arg}(b_1^\pm)$  which in general may be different for the two valleys. These expressions clearly show that far from the interface in CR currents of both valleys have the same direction determined by the sign of  $k_y$ . In figure(2c) sum of the two currents is plotted which shows that angular symmetric incidence of the particles of the two valleys will result in no net charge current just like the case of common systems,

however, of course, there will be two non-zero valley currents flowing in opposite directions.

Let's summarize above findings and draw some conclusions. We see that the wavefunction matching conditions remain the same in case of energy dependant effective mass in gaped bilayer graphene system which is very unusual. We showed that the states localized near an interface between conducting and insulating regions of BLG on the insulating side despite having plane wave parts along the decay direction carry no currents along it. Further, we have seen that their properties in transverse direction are strikingly different than those of evanescent waves in ordinary systems where direction of current follow the sign of corresponding wavevector component. Moreover, the states belonging to the two valleys show contrasting behavior and their presence also modifies the properties of the localized states on the conducting side of the interface. Their valley dependent properties are insensitive to various mechanisms that can possibly pose problems for earlier proposals to obtain basic valley based functionalities. They are easy to exploit in realistic situations to obtain valley polarization, filter particles of a desired valley or for valley switching *without* dealing with the propagation angles of the particles or facing any other experimental challenges. Thus we expect them capable of playing an important role in valleytronics based on bilayer graphene system.

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**Figure captions:**

**Fig.1**(color online). Variation of currents  $J_y^\pm$  of the two valleys  $K(+)$  and  $K'(-)$  with distance from the interface  $x$  and component of wavevector along the interface  $k_y$ . Figure shows that for a given polarity of gates  $J_y^+$  and  $J_y^-$  have fixed opposite directions that do not depend on the sign of  $k_y$ . **(a)**  $J_y^\pm$  for  $U = \pm 50 meV$  **(b)**  $J_y^\mp$  for  $U = \pm 50 meV$  and **(c)** sum of the two currents  $J_y^\pm$ ,  $J_y^+ + J_y^-$  for  $U = \pm 50 meV$ . From the figure the width of the region that supports the valley polarized currents along the fixed directions is roughly  $15 nm$ .